Further study of the Over-Barrier Model to compute charge exchange processes

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Abstract

In this work we present an improvement over the Over Barrier Model (OBM) described in a recent paper [F. Sattin, Phys. Rev. A **62**, 042711 (2000)]. We show that: i) one of the two free parameters there introduced actually comes out consistently from the starting assumptions underlying the model; ii) the modified model thus obtained is as much accurate as the former one. Furthermore, we show that OBMs are able to accurately predict some recent results of state selective electron capture, at odds with what previously supposed.

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The electron capture process in collisions of slow ions with neutral atoms or other ions is of great importance in basic atomic physics, plasma physics and astrophysics. In principle, one could compute all the quantities of interest in such processes by writing the time-dependent Schrödinger equation for the system and programming a computer to solve it. This task can be performed on present–days supercomputers for moderately complicated systems. Notwithstanding this, simple approximate models are still valuable: (i) they allow getting analytical estimates, which are easy to adapt to particular cases; (ii) allow getting physical insight on the features of the problem by looking at the analytical formulas; (iii) finally, they can be the only tools available when the complexity of the problem overcomes the capabilities of the computers. For this reason new models are being still developed [1–3].

The present author has presented in a recent paper [4] a study attempting to improve an already existing OBM [2] (this model will be hereafter referred to as I). The model there developed is able to predict cross sections for electron capture and ionization with appreciable accuracy for a large number of test cases. The key element was found to be the inclusion within the model of two free parameters, there labeled α and f_T. A large part of the paper [4] was devoted to show that, more than simple adjustable parameters, α and f_T stand for some physical mechanism still not adequately included within the model. As such, one should expect they retain constant values from case to case, or vary according to some well defined relationship with the parameters of the problem at hand. Actually, it was found, by applying the model to a number of test cases, that a good agreement with experiment and/or other computations was obtained always with the same choice for both parameters (in detail, $\alpha = 1$, $f_T = 2$).

In this paper we show that a correction to the capture probability, having the same meaning of parameter f_T, should appear naturally within the frame-

work of the model I; that in the work [4] it was incorrectly overlooked and, as a consequence, we were forced to insert f_T by hand in order of recovering accuracy of the results.

Let us begin with a brief summary of model I; the reader is referred to [4] for a more complete discussion. We consider a standard scattering experiment between a target nucleus **T** and a projectile nucleus **P** with only one active electron **e**. We are considering hydrogenlike approximations for both the target and the projectile. Let **r** be the electron vector relative to **T** and **R** the distance between **T** and **P**. In the spirit of classical OBMs, all particles are considered as classical objects.

Let us consider the plane $\mathcal{P}$ containing all the three particles and use the projection of cylindrical polar coordinates $(\rho, z, \phi \equiv 0)$ to describe the position of the electron within this plane. We can assign the z axis to the direction along the internuclear axis.

The total energy of the electron is (atomic units will be used unless otherwise stated):

$$E = p^2 2 + U = p^2 2 - Z_t\sqrt{\rho^2 + z^2} - Z\sqrt{\rho^2 + (R-z)^2} \quad . \tag{1}$$

Z and Z_t are the effective charge of the projectile and of the target, respectively. From here on, we assign an effective charge $Z_t = 1$ to the target and an effective quantum number n to label the binding energy of the electron: $E_n \equiv 1/(2n^2)$.

When the projectile approaches the target nucleus, it also contribute to increase (in absolute value) the binding energy of the electron: for distant encounters, we can approximate E as

$$E(R) = -E_n - ZR \quad . \tag{2}$$

On the plane $\mathcal{P}$ we can draw a section of the equipotential surface

$$U(z, \rho, R) = -E_n - ZR \quad . \tag{3}$$

This represents the limit of the region classically allowed to the electron. When $R \to \infty$ this region is divided into two disconnected circles centered on each of the two nuclei. Initial conditions determine which of the two regions actually the electron lives in. As R diminishes there can be eventually an instant where the two regions become connected. See fig. (1) of [4] for an example of this.

In the spirit of OBMs it is the opening of the equipotential curve between **P** and **T** which leads to a leakage of electrons from one nucleus to another, and therefore to charge exchange. It is easy to solve eq. (3) for R by imposing a vanishing width of the opening:

$$R_m = (1 + \sqrt{Z})^2 - ZE_n \quad . \tag{4}$$

In the region of the opening the potential U has a saddle structure. Charge loss occurs provided the electron is able to cross this potential barrier. Let N_Ω be the fraction of trajectories which lead to electron loss at the time t. An approximate expression (valid for distant collisions) for N_Ω is given in [2]. We simply quote that result:

$$N_\Omega \approx 12\sqrt{Z}(\sqrt{Z}+1)^2 \left[(\sqrt{Z}+1)^2 - Z - E_n R\right] \quad . \tag{5}$$

The leakage probability is related to N_Ω through

$$P_l = 1 - \exp\left(-f_T T \int_{-t_m}^{+t_m} N_\Omega dt\right) \quad . \tag{6}$$

In this expression dt/T is the fraction of electrons which cross any surface perpendicular to their motion (and enter the loss region) within time interval dt, with $T = 2\pi n^3$ the unperturbed period of the electron motion along its orbit, and f_T a corrective term which accounts for the perturbation.

In order to actually integrate Eq. (6) we need to know the collision trajectory; for this an unperturbed straight line with b impact parameter is assumed:

$$R = \sqrt{b^2 + (vt)^2} \quad . \tag{7}$$

The extrema $\pm t_m$ in the integral (6) are the maximum values of t at which charge loss can occur. They are related through Eq. (7) to the maximum distance at which capture may occur, R_m (Eq. 4). This is the original estimate for R_m as given in [2]. In [4] this estimate was questioned on the basis of the fact that it overestimated the maximum impact parameter available for charge exchange as computed by Classical Trajectory Monte Carlo (CTMC) calculations. As a consequence, the cross sections were overestimated, too. To remedy this, in [4] it was suggested to replace Eq. (4) with

$$R'_m = (\alpha\sqrt{Z} + 1)E_n \quad . \tag{8}$$

With the choice $\alpha = 2$ we recover Eq. (4), but it was found that better agreement with data was obtained for $\alpha = 1$. The value $\alpha = 1$ can be given also a physical meaning: it is easy to show (see for details ref. [4]) that, when substituted into Eq. (8), it yields the maximum distance at which an electron can be captured provided that, prior to the capture, the electron trajectory is not perturbed in any way by the projectile, i.e. the electron follows a trajectory with constant energy $E = -E_n$, instead of E given by eq. (2).

We can write, after all this,

$$\begin{aligned} &\int_{-t_m}^{t_m} N_\Omega dt = 2F\left(vt_m b\right) \\ &F(u) = \sqrt{Z}2(\sqrt{Z}+1)^2\left[\left((\sqrt{Z}+1)^2 - Z\right)bvu - \left(E_n b^2 2v\right)\left(u\sqrt{1+u^2} + \operatorname{arcsinh}(u)\right)\right] \quad . \end{aligned} \tag{9}$$

The cross section can be finally obtained after integrating over the impact parameter (this last integration must be done numerically):

$$\sigma = 2\pi \int b P_l(b) db \quad . \tag{10}$$

The integration extends till the maximum b allowed: $b_m = R'_m$.

The key point we want to underline here is that the definition of the orbital period given above is not consistent with basic hypotheses (2): it is based in fact on the relation for the periodic motion along the radial direction [5]:

$$T = 2\int_0^{1/E} drp = \sqrt{2}\int_0^{1/E} dr\sqrt{1r - E} \quad . \tag{11}$$

One recovers $T = 2\pi n^3$ by putting $E \equiv E_n$ in this equation. However, to be consistent with Eq. (2) one should assume that the orbital period of the electron is changed, just like its binding energy, while the projectile is approaching. The expression Eq. (2) should thus be used in (11). By doing so, one gets

$$T' = 2\pi \left[2\left(E_n + ZR\right)\right]^{-3/2} = T\left[1 + ZE_nR\right]^{-3/2} \tag{12}$$

The orbital period is now a varying quantity function of time, and it is always $T' < T$. The exact value of the enhancement factor T/T' depends upon R. In [4] this enhancement factor was held constant, being the parameter f_T, usually taken equal to 2. In order to have a quantitative estimate let us remark that captures occur preferentially for R of order of R'_m (see e.g. fig. 5 of ref. [4]). We replace therefore R with R'_m in the previous equation and get that T/T' reaches its minimum value $T/T' = (3/2)^{3/2} \approx 1.84$ for $Z = 1$ (with $\alpha = 1$). The ratio increases rather slowly with Z: asimptotically it follows the scaling $T/T' \approx Z^{3/4}, Z \to \infty$; however, it is already $T/T' > 2$ for all integer values $Z > 1$. Therefore, we expect to have enhanced cross sections with respect to model I when dealing with highly charged projectile ions, while they should be-very slightly-depressed in collisions with singly charged ions. This is a confirmation of the guess done in [4], according to which f_T was likely to be an increasing function of Z.

Equation (6) must therefore be rewritten (without the factor f_T):

$$P_l = 1 - \exp\left(-\int_{-t_m}^{+t_m} N_\Omega T' dt\right) \quad . \tag{13}$$

Unfortunately, the integral in (13) can no longer be computed analytically; however, σ is still easily numerically computed with only a few lines of code written in any mathematical software package.

We want now to test the model: as a first test case we address the process

$$\mathrm{H} + \mathrm{Be}^{4+} \rightarrow \mathrm{H}^{+} + \mathrm{Be}^{3+} \quad . \tag{14}$$

It has been studied by two different approaches in [6,7], so we can rate predictions of Eqns. (6,13) against some sophisticated theories. The results are plotted in fig. (1). The agreement between the old and the new model is rather good, with the latter slightly overestimating the former, as expected.

As a second test case we present the results for collisions H^{+}– Na(3s,3p) (fig. 2). Here the projectile is singly charged, so Eq. (13) is expected to give a result lower than Eq. (6), and this is exactly found. In this case, as already remarked in [4], the performance of the model is rather bad. We can just state again that the reason could be found in the non-hydrogen-like nature of the target. An upgrade of the model taking into account more realistic model potentials binding the electron could give remarkable enhancements.

We want now to address a rather different point. It is partially unrelated with previous topics since it does not deal with any kind of improvement to the model. Instead, we will show that the OBM (any version of it, be the original version by Ostrovsky, the version I or the present one) is able to predict some experimental results previously thought not amenable to this kind of analysis. The experiments we are referring to, on charge exchange between slow ions and Rydberg atoms, are reported in the paper [9]. Among other quantities, it was measured the binding energy of the captured electron

E_p as a function of the impact velocity v, of the projectile charge Z_p and–above all–of the binding energy of the Rydberg target E_t, which allowed to compute the normalized energy defect function $1-k=(E_p-E_t)/E_p$. This is a convenient quantity since it can be computed for a number of models, including the CTMC method and OBMs. Within the OBM the computation goes as follows: the initial energy of the electron is $E=-E_t-Z/R$ whereas in the final state it is $E=-E_p-1/R$. When the electron is being transferred from one nucleus to the other the two quantities must be equal, thus

$$\begin{aligned} & E_t+ZR=E_p+1R\rightarrow \\ & 1-k\equiv E_p-E_tE_p=Z-1Z-1+E_tR \quad . \end{aligned} \tag{15}$$

The maximal contribution to charge exchange is given by R close to the maximum allowed R'_m (see e.g. fig. 4 of [2] or fig. 5 of [4]). Therefore we set $R=fR'_m$. f is a factor as yet undetermined accounting for the fact that the maximum is not exactly at R'_m but at slightly lower values. Replacing this expression in (15) we get

$$1-k=Z-1Z-1+f(\alpha\sqrt{Z}+1) \quad . \tag{16}$$

Naively, one could set $f=1$ and get

$$1-k=Z-1Z+2\sqrt{Z} \tag{17}$$

(where we have also set $\alpha=2$). This is the estimate for $1-k$ as given in [9] and also in [2,10]. The previous formula gives poor estimates for the experimental results and in [9] it was suggested that the failure was due to the approximations intrinsic to OBMs. We shall see, instead, that a little refinement to the above analysis gives us a rather good agreement with experiment. We exploit the extra degree of freedom given by f: a reasonable choice for f is to choose the value of R at which the capture cross section has a maximum and set $f=R/R'_m$. It is more convenient, although lesser accurate, to look

for the maximum in $bP(b)$ as a function of b. Since the equation $d(bP)/db = 0$ cannot be solved analitically we resort to a backward procedure: determine by a least squares fit the value of f which best interpolates the data and check if this value corresponds to the maximum in bP. In fig. (3) we plot the experimental data from ref. [9], the naive expression (17), and the above mentioned fits. Computations have been repeated for the two couples of parameter $\alpha = 1, f_T = 2$ and $\alpha = 2, f_T = 1$. For the computation of P we have used expression (6): using Eq. (13) would be a pointless complication.
Both fits are fairly good, although obtained with widely different values of f: the choice $\alpha = 1$ imposes $f = 0.802$, while $\alpha = 2$ yields $f = 0.492$. In fig. (4) we plot the corresponding differential cross sections. The maximum of bP is only faintly a function of the projectile charge. The case $\alpha = 2$ gives a very good accordance between the fit and the actually computed differential cross sections; thus, in this case, we can definitely state that the OBM is able to predict the results of [9]. The case with $\alpha = 1$ is slightly worse: the maximum of the cross section is around $0.65 \div 0.7$.

To summarize, being able to justify one apparently free parameter from within the framework of the model itself is reassuring about its validity and its ability of catching as much physics of the capture process as possible. On the other hand, rather paradoxically, this makes even more puzzling the presence of the remaining free parameter, α. We remind in fact that the choice $\alpha = 2$ should be the correct one, in that it is consistent with the same starting hypotheses which allow us to arrive at Eq. (12). It is however necessary using $\alpha = 1$ to be consistent with CTMC simulations, even though this means that we are making the same kind of error done when using T instead of T'
We have not at the moment a satisfactory explanation to this problem. It is not unlikely, however, that the ultimate reason lies in the failure of expression (2) for the electron energy E close to the saddle point. That expression,

in fact, holds rigorously only for large electron-projectile distances. At the saddle point, instead, the electron-target and electron-projectile distances are equivalent.

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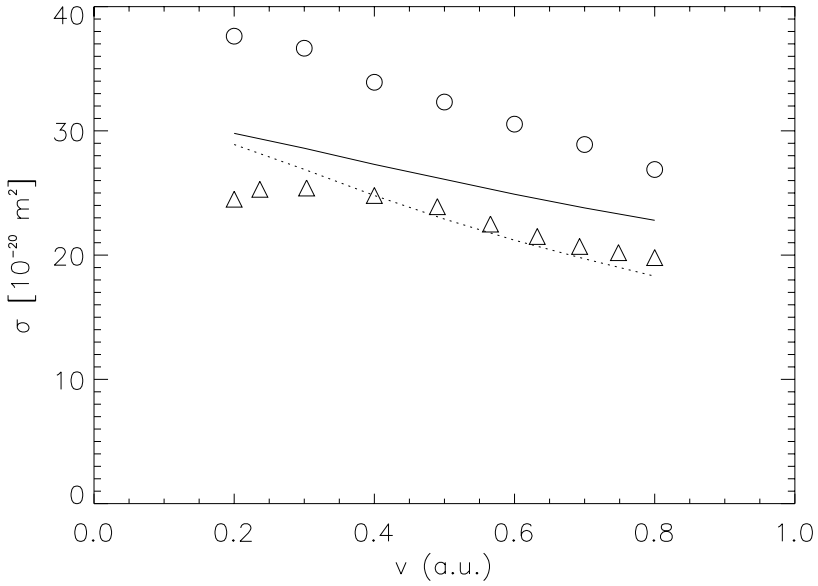

FIG. 1. Charge exchange cross section versus velocity for Be^{4+}-H(1s) collisions. Triangles, data from ref. 6; circles, data from ref. 7; solid line, present model using $\alpha = 1$; dotted line, model I using $\alpha = 1, f_T = 2$

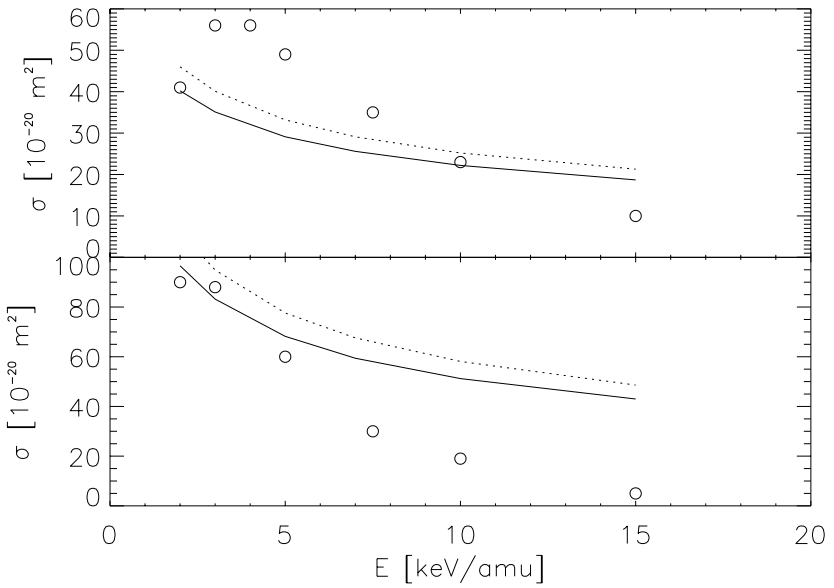

FIG. 2. Cross section for charge exchange in H^+–Na(3s) (upper) and H^+–Na(3p) (lower) collisions. Symbols, experimental data from ref. 8; solid line, present model; dotted line, model I.

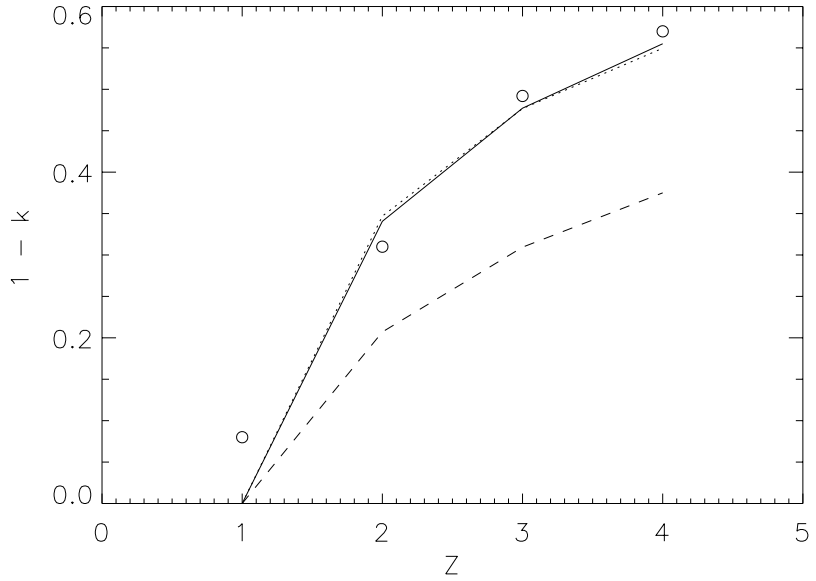

FIG. 3. Normalized energy defect as a function of projectile charge. Symbols, data from ref. 9; dashed line, OBM prediction from Eq. (17); dotted line, least squared fit to data using Eq. (16) and $\alpha = 1$; solid line, least squares fit to data using Eq. (16) and $\alpha = 2$.

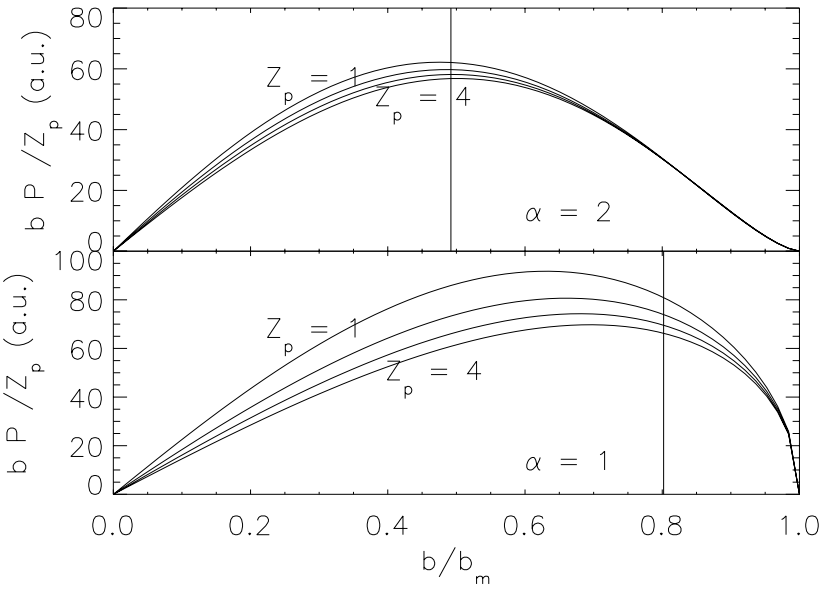

FIG. 4. Scaled differential cross section $bP(b)/Z_p$ *versus* scaled impact parameter for the choices $\alpha = 2, f_T = 1$ (upper) and $\alpha = 1, f_T = 2$ (lower) and different projectile charges. The position of the maxima of the cross section as estimated by the least squares fit done using Eq. (16) are shown.